Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries

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Ford Motor Company

2018 DOE Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting
Jun 20th, 2018

Project ID # BAT296

Overview

Timeline

- Start: Jan 1, 2016
- End: Dec 31, 2018
- Percent completion: 70%

Barriers Addressed

- Battery/Energy Storage R&D
  - Development Cost
  - Abuse tolerance and reliability

Budget

- Total contract value: $4.375M
  - $3.5M DOE/TARDEC share
  - $875k Ford share
- Funding received in 2017: $856k (EERE)
- Funding for FY 2018: $1.188M (EERE)

Partners

- Oak Ridge National Laboratory (ORNL) & Livermore Software Technology Corporation (LSTC)
- Project Lead: Ford Motor Company

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Relevance

- **Project Objective**
  - Develop a simulation tool to predict the combined structural, electrical, electrochemical, and thermal (EET) responses of automotive batteries to crash-induced crush and short circuit, overcharge, and thermal ramp and validate it for conditions relevant to automotive crash.

- **Barriers Addressed**
  - Cost
    - Cost reduction by shortened development cycle and optimized crash protection systems.
    - Avoid late-cycle design changes due to regulatory requirement change (i.e. regulatory crush, > 10 s vs. Crash, < 100 ms).

  - Abuse tolerance
    - Improvement in abuse tolerance of a battery by delivering a predictive simulation tool to shorten or eliminate design – build – test prototype cycles.
    - Accelerating optimization of crash protection systems being more robust to the safety requirements.

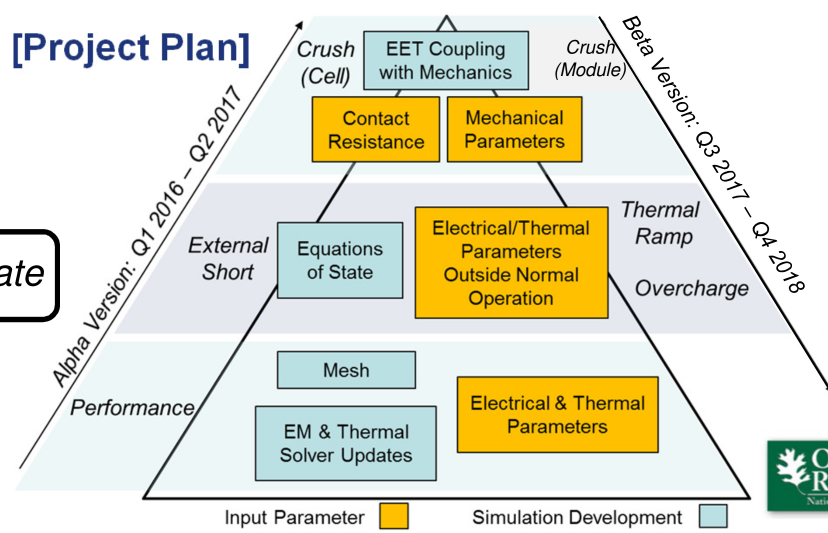
Go Further

Approach and Milestones

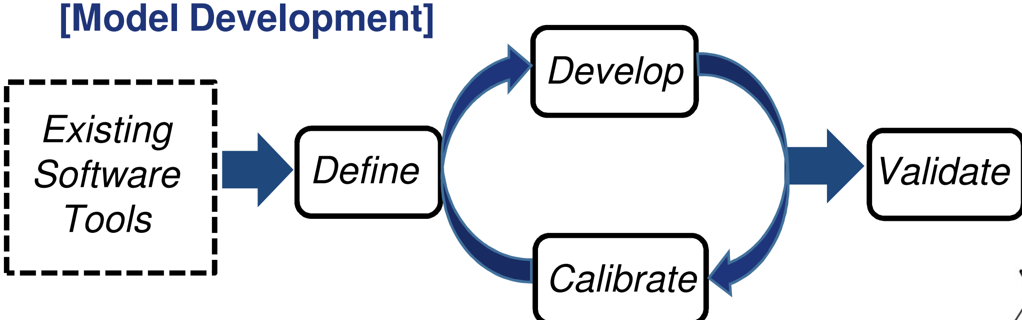
[Milestones]

Tasks	2016 Q1	2016 Q2	2016 Q3	2016 Q4	2017 Q1	2017 Q2	2017 Q3	2017 Q4	2018 Q1	2018 Q2	2018 Q3	2018 Q4
Hardware selection for Alpha version	■											
Development assumptions for Alpha version	■	■										
Alpha version multi-physics solvers and material models (EM & Therm)		■	■	■	■	■						
Alpha version model inputs		■	■	■	■	■						
Integrate solvers into Alpha version				■	■	■						
Validation of Alpha version			■	■	■	■	■	■				
Development assumptions for Beta version							■					
Hardware selection for Beta version							■	■	■			
Beta version multi-physics solvers and material models								■	■	■		
Beta version model inputs									■	■	■	■
Integrate solvers into Beta version											■	
Validation of Beta version									■	■	■	■

[Project Plan]



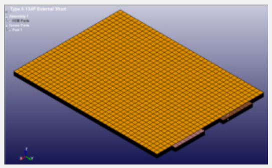
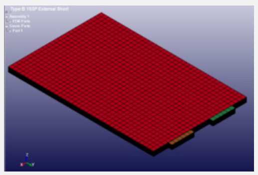
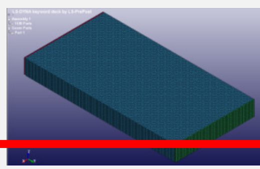
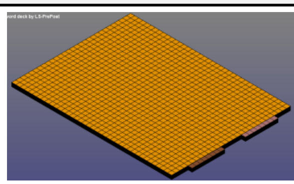
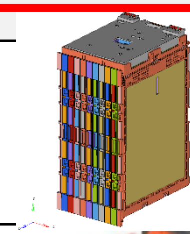
[Model Development]



Go Further

Technical Accomplishments: Hardware Selection

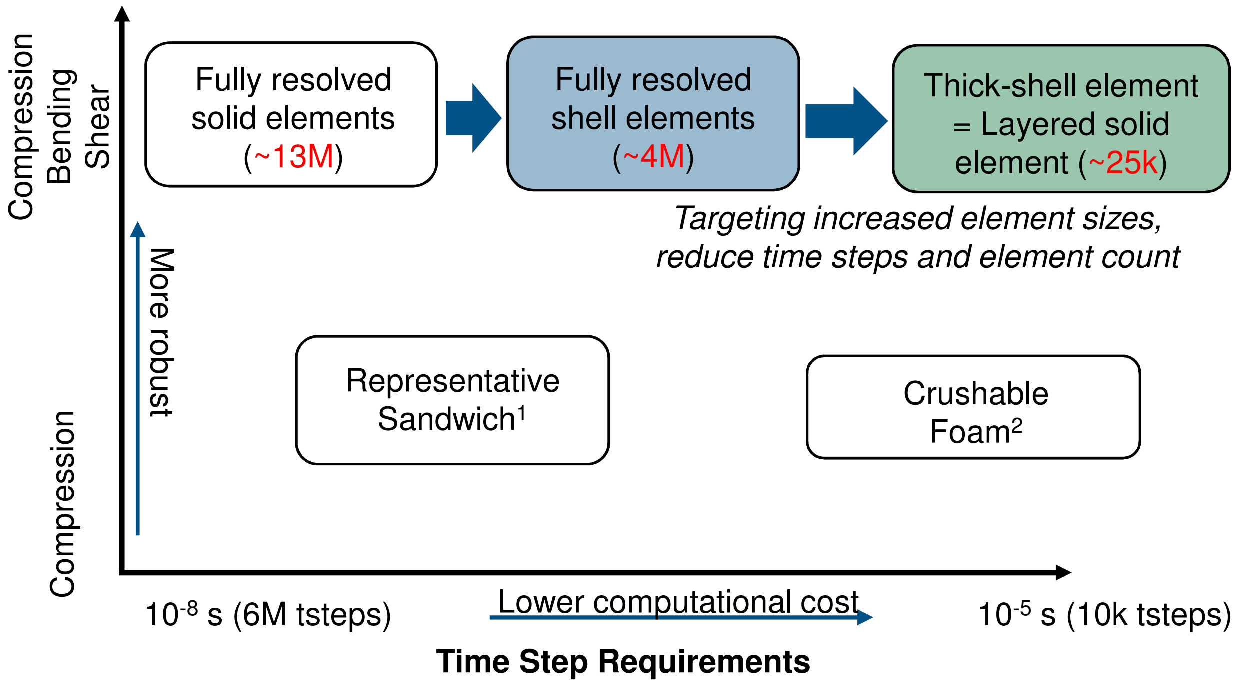
Type D and Type E modules were selected in 2017 for β-model development

Mesh/Geometry	Type	Cathode Chemistry and Format	Cell	Module	Pack
	A	NMC//LMO Blend Pouch	15 Ah 3.7 V 0.06 kWh	4P1S 5P4S	4S5P (x9) + 2S5P (x2)
	B	NMC Pouch	20 Ah 3.6 V 0.07 kWh	3P1S and 3P10S	
	C	LFP Prismatic	18 Ah 3.2 V 0.06 kWh	4P1S 5P2S	36S5P
	D	NMC Pouch	21 Ah 3.65 V		4S5P (x9) + 2S5P (x2)
	E	Metal Oxide Blend Prismatic	63 Ah 3.65 V (est)		1P5S (X11) + 1P6S (X7)

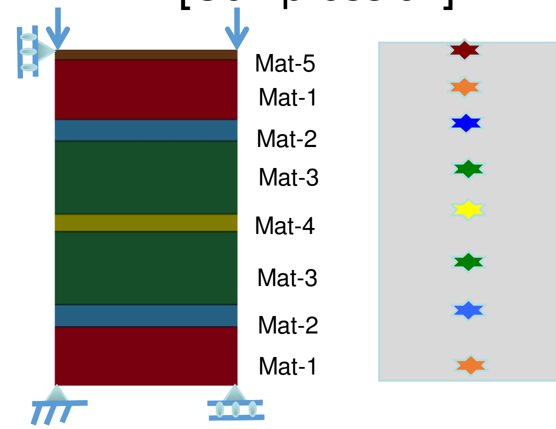
Legacy Hardware ☐ Hardware sourced for this project ☐

Go Further

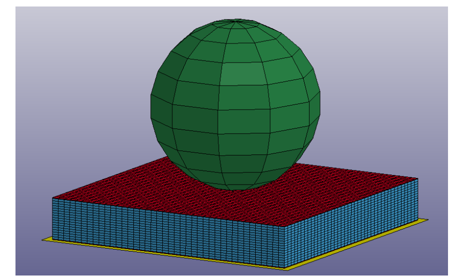
Technical Accomplishment: Major Accomplishment In Previous Year
Development of Layered Solid Element Solver



[Compression]



[Indentation]



- **Layered solid solver was developed and verified by comparing its performance to solid element solver's under three deformation modes (compression, indentation, and bending modes)**
  - Solid element solver was developed and calibrated using legacy cells' input parameters and empirical data for previous project.
  - Same information was used to verify performance of layered solid element solver against that of proven solid element solver under three different deformation modes.
  - It was observed that the layered solid element provided the same results but much faster computational time compared to solid element (i.e. 105 times faster for indentation).

Technical Accomplishment: Major Accomplishment In 2017 Development of α-Version Model

	2017			
Tasks	Q1	Q2	Q3	Q4
Alpha version multi-physics solvers and material models (EM & Therm)				
Alpha version model inputs				
Integrate solvers into Alpha version				
Validation of Alpha version				
Development assumptions for Beta version				
Hardware selection for Beta version				
Beta version multi-physics solvers and material models				

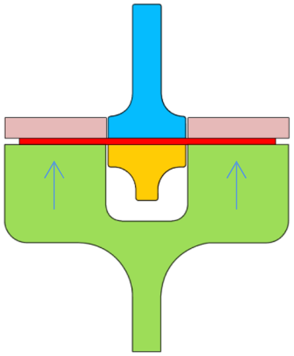
- **Layered solid element solver was further developed and calibrated with various materials models.**
- **EM (Electro Magnetic) and thermal models were developed and calibrated.**
- **New solver and α-version multi-physics model were developed and verified with empirical data from the following tests;**
  - Shear stress tests (representing shear stress mode).
  - Quasi-static tests (compression bending and indentation modes).
  - High speed impact tests (compression bending and indentation modes).

Technical Accomplishment: Shear Stress Test Setup

- **Tested Cell SOC at 0 % (~2.92 V) to eliminate any thermal event for;**
  - Safely conducting the experiments.
  - Post-mortem analyses with a 3D X-ray CT (Computed Tomography) scans.
- **Shear test fixtures: (a) load frame (b) shear fixture (c) shear fixture and force direction.**

(a)

(b)

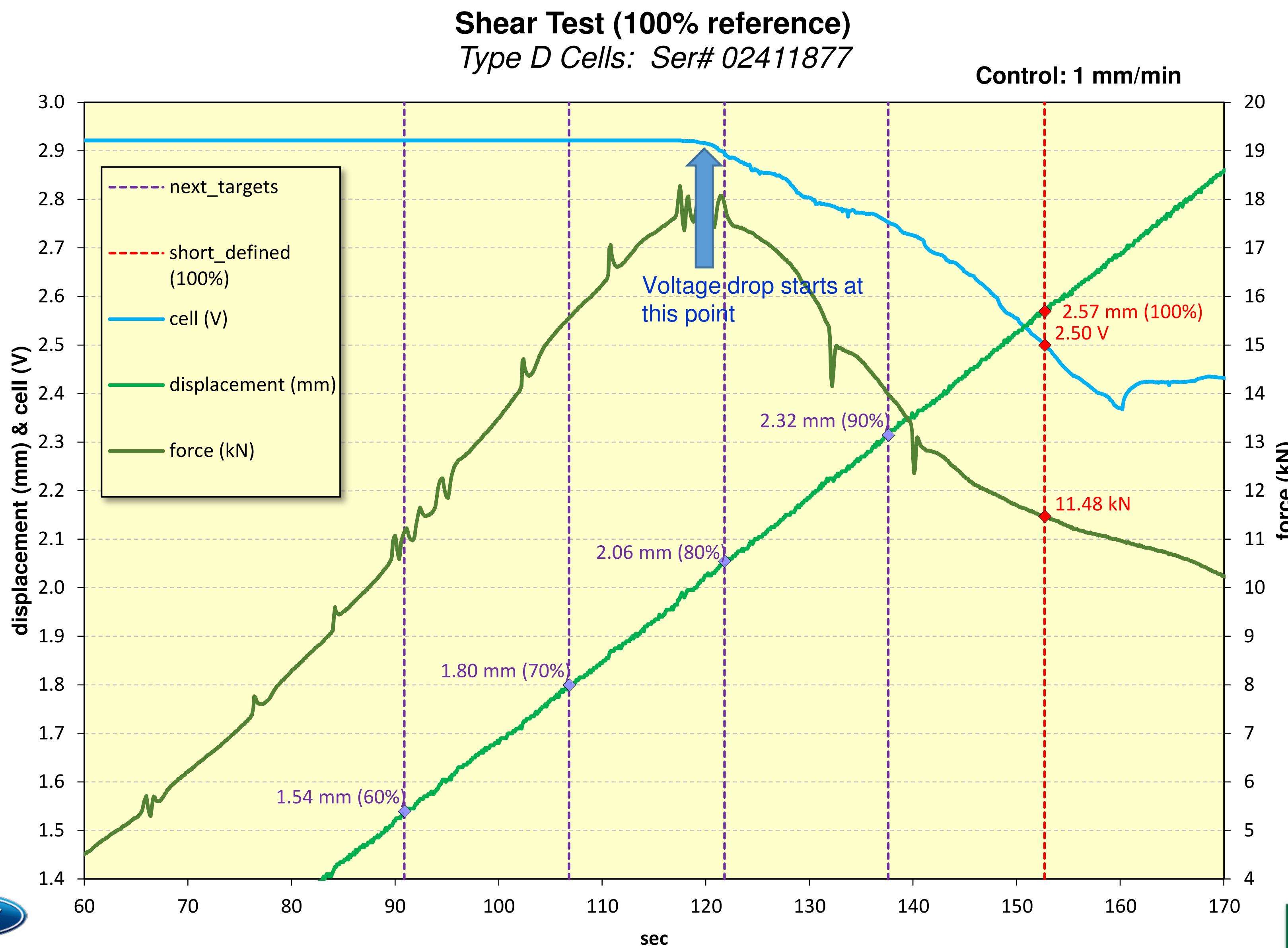


(c)

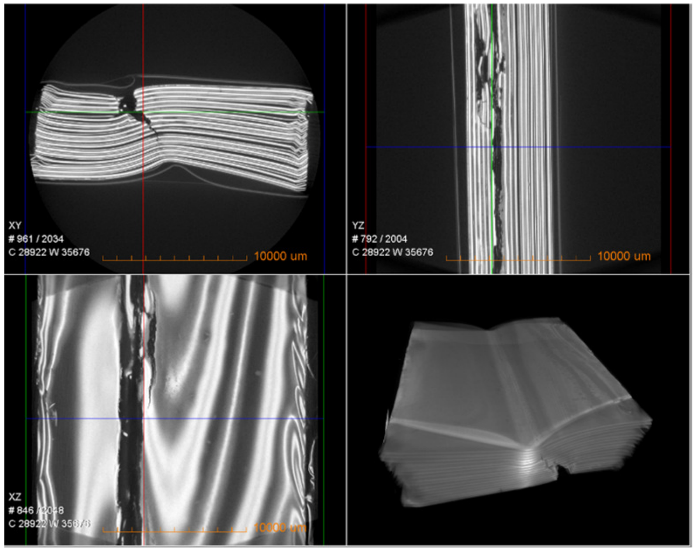
- **Run successive tests with Type D cells at the different displacements to analyze onset of crack formation and growth on cell components.**
  - 100% displacement was defined by voltage drop by 0.5V.
  - Next 10% displacement was calculated by 90% of the previous displacement (i.e. 100% displacement→ 3 mm, 90% displacement → 2.7 mm).
- **During tests, cell voltage, displacement, and force were recorded.**
- **X-ray CT scan results would be used to develop the failure models.**

Go Further

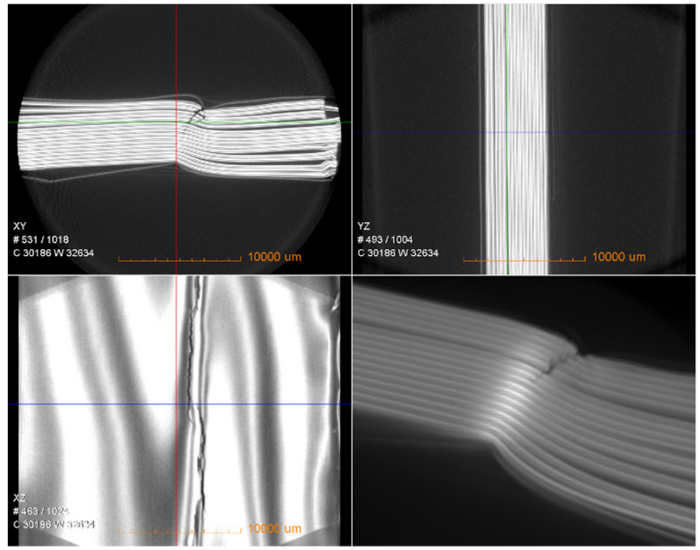
Technical Accomplishment: Type D Cell Shear Stress Test for 100 % Displacement (Reference)



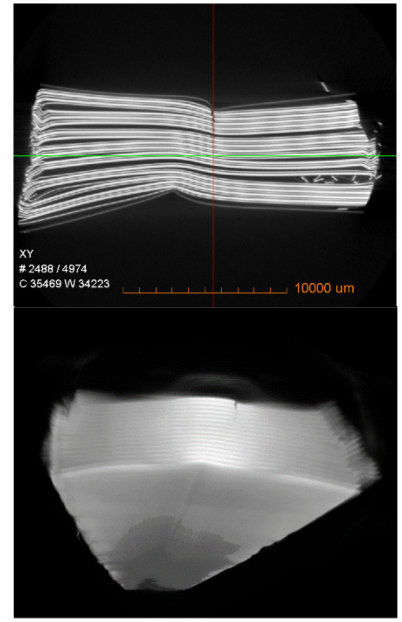
Technical Accomplishment: X-Ray CT Scan Analyses of Type D Cell Shear Stress Test for 100 % ~ 80% Displacements



[100% Displacement]



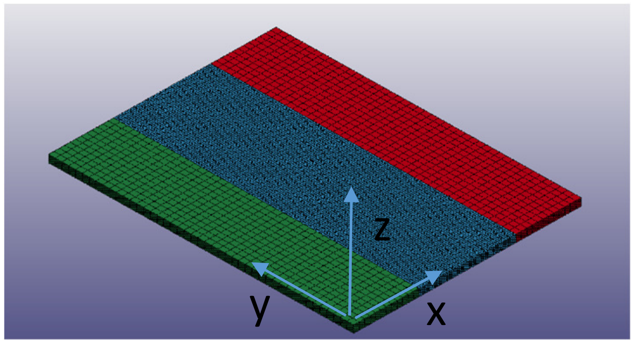
[90% Displacement]



[80% Displacement]

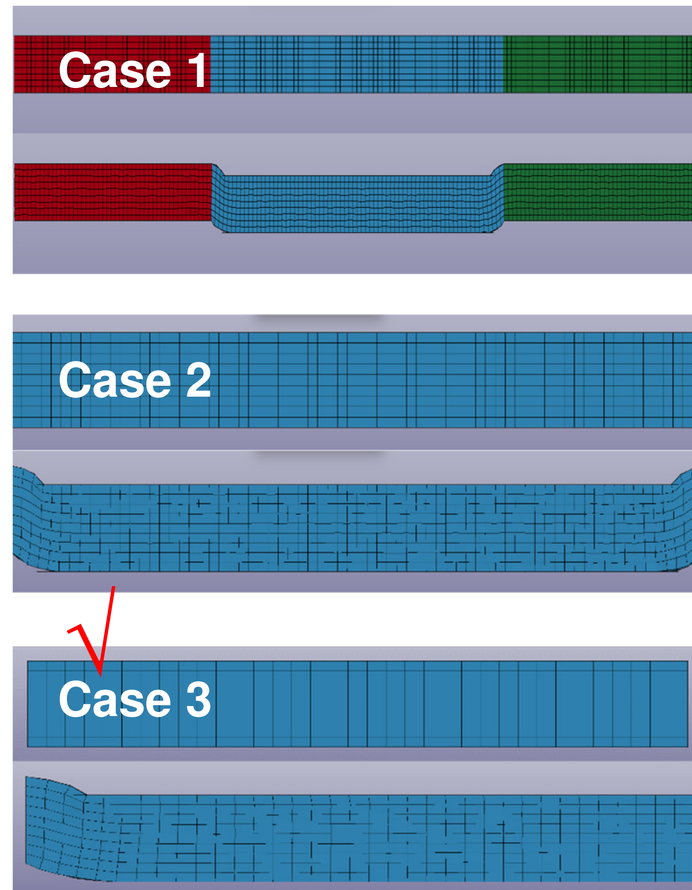
- **Cell marked 70% did not have any noticeable cracks.**
- **In the summary test graph, it seems that the voltage starts dropping close to 80% mark, which may indicate internal crack formation (see page 9).**
- **We are expecting that due to the material composition the crack occurs across several layers, which may be also indicated by noticeable change in the potential curve slope (see page 9).**

Technical Accomplishment: Layered Solid Solver – Type D Cell Meshed Cell and Different Ways to Model the Cell for Shear Tests



- **Parts of the cell represented by red and green colors are clamped, and the blue region is displaced in the vertical direction under shear test.**

- **Case 1: Top and bottom nodes in the red and green regions are fixed in all directions and blue region is displaced in X-direction using flat plates.**
- **Case 2: Nodes on the left and right YZ surfaces of the blue region are fixed, and the remaining blue region is displaced using flat plates.**
- **Case 3: Only one half of the blue region is considered. Nodes on the left YZ surface are fixed in all directions. On the right YZ surface, symmetric boundary conditions are applied such that nodes are allowed to move in Z-direction only.**
  - Case3 has least number of degree of freedom, so for computational efficiency it makes sense to use this for analysis.



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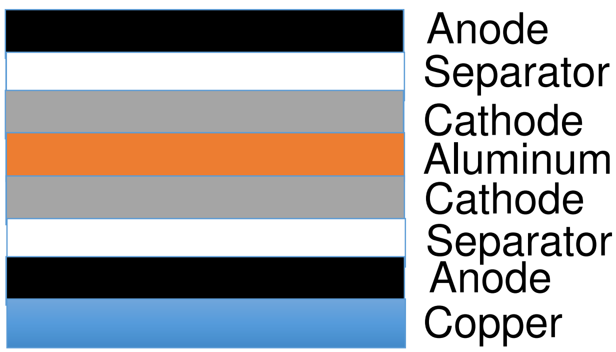
Technical Accomplishment: Layered Solid Solver – Unit cell details and Parameters for Each Component of Type D Cell

- **Total 72 layers of cathode, anode and separator, 36 layers of current collector**

18 element across thickness



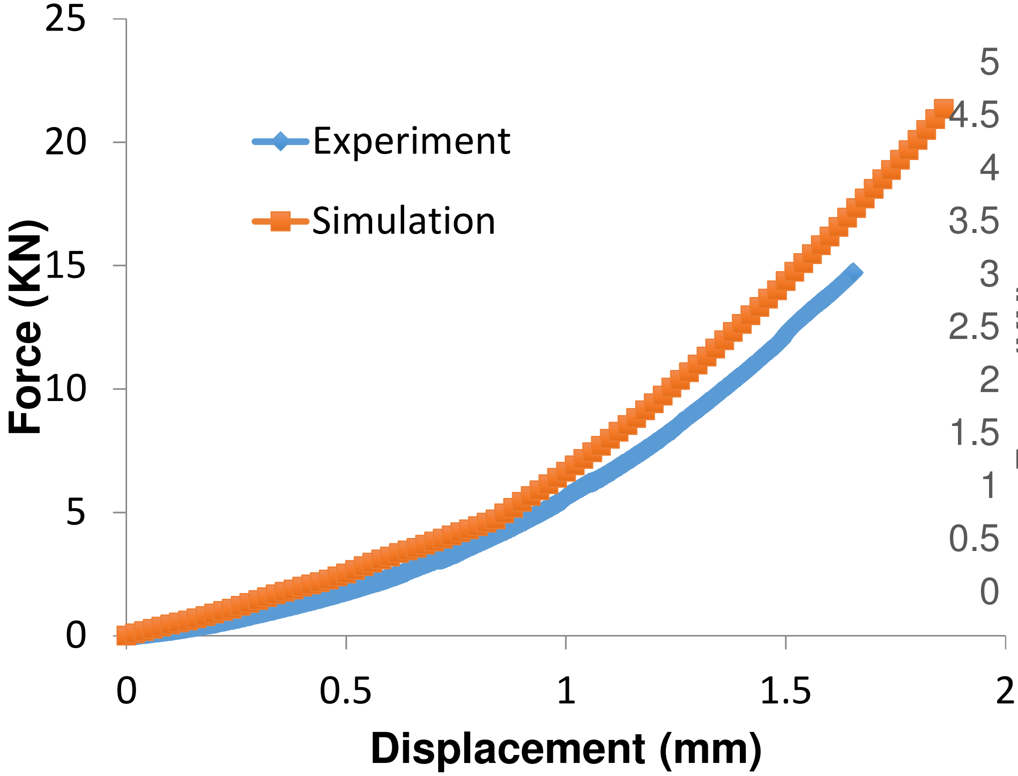
- Element Thickness = 0.304 mm
- 8 integration point in the element

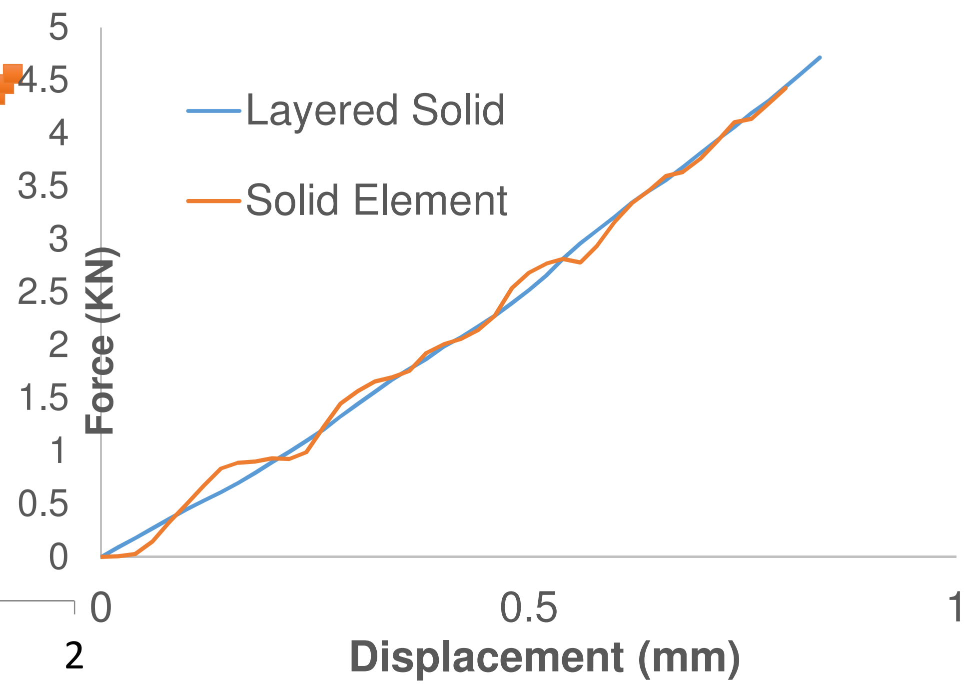
- **Anode and cathode are represented by MAT-63 material model.**
- **Other component are represented by Material Model MAT-24.**

Component	Thickness (mm)	Elastic Modulus (Gpa)	Yield Strength (Gpa)	Tangent Modulus (Gpa)
Anode	0.064	0.45		
Separator	0.023	0.50	0.045	0.01
Cathode	0.053	0.55		
Aluminum Current Collector	0.015	70	0.24	0.1
Copper Current Collector	0.009	110	0.24	0.1

Go Further

Technical Accomplishment: Layered Solid Solver Experiment vs. Simulation and Solid Element vs. Layered Solid





Number of Solid Element = 9504
Aspect Ratio Solid Element = 111.1
Computation Time Solid Element = 10740 sec

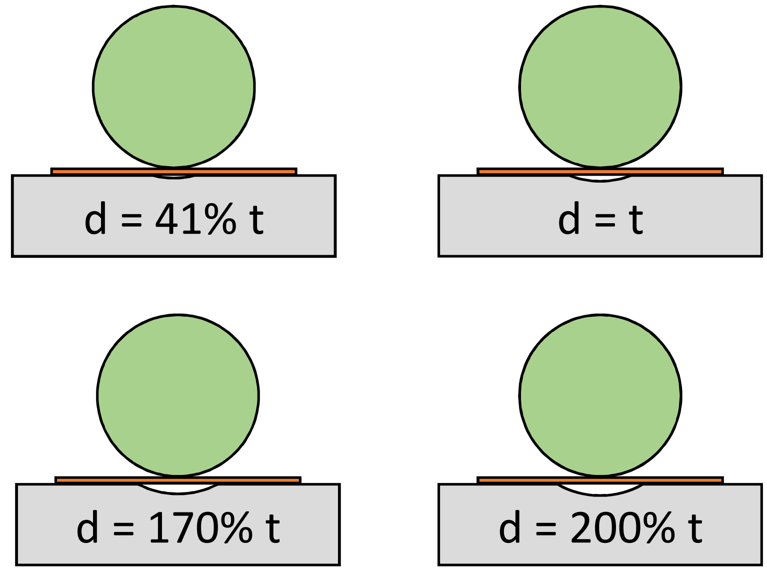
Number of Layered Solid Element = 1188
Aspect Ratio Layered Solid = 3.33
Computation Time Layered Solid Element = 554 sec

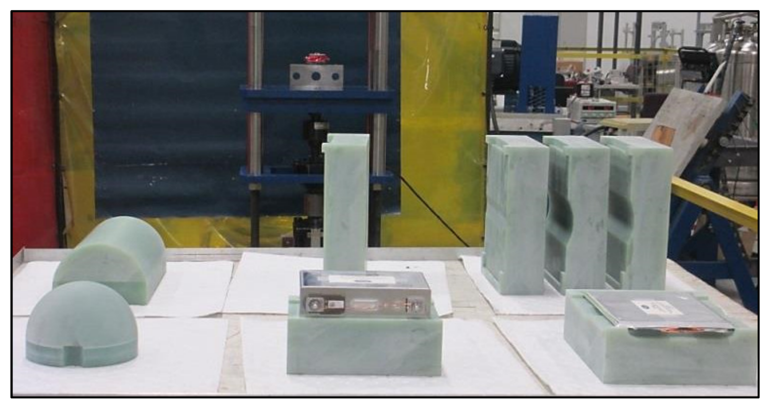
Go Further

Technical Accomplishment: Quasi-Static Test Matrix

Quasi-static				
Test Number	Type	Orientation	Indenter Shape	Repetition
1	D	Flat	Cylinder	1
2	D	Flat	Cylinder	2
3	D	Flat	Cylinder	3
4	D	Bending (d=200%t)*	Cylinder	1
5	D	Bending (d=200%t)	Cylinder	2
6	D	Bending (d=200%t)	Cylinder	3
7	D	Bending (d=170%t)	Cylinder	1
8	D	Bending (d=170%t)	Cylinder	2
9	D	Bending (d=170%t)	Cylinder	3
10	D	Bending (d=t)	Cylinder	1
11	D	Bending (d=t)	Cylinder	2
12	D	Bending (d=t)	Cylinder	3
13	D	Bending (d=41% t)	Cylinder	1
14	D	Bending (d=41% t)	Cylinder	2
15	D	Bending (d=41% t)	Cylinder	3
16	D	Flat	Sphere	1
17	D	Flat	Sphere	2
18	D	Flat	Sphere	3
19	E	Flat	Cylinder	1
20	E	Flat	Cylinder	2
21	E	Flat	Cylinder	3
22	E	Flat	Sphere	1
23	E	Flat	Sphere	2
24	E	Flat	Sphere	3
Total				**24**

[Compression-bending test hardware orientations]

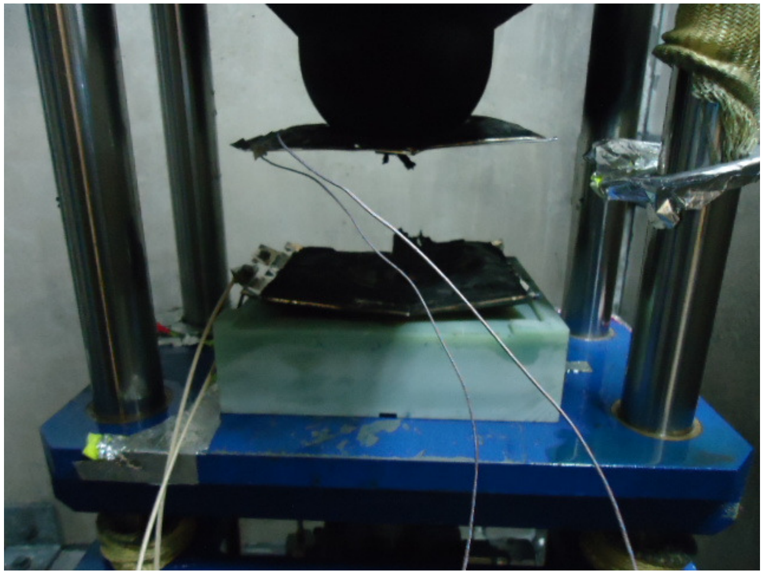




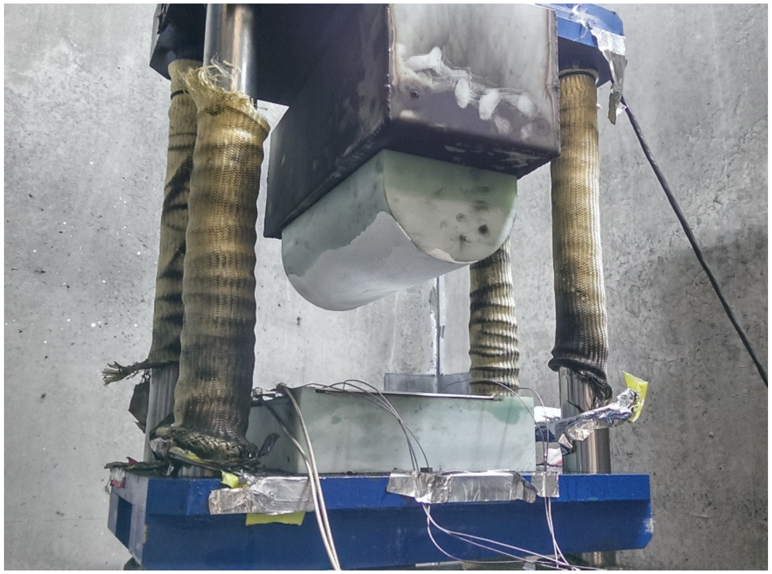
FR4 indenters and platens

Technical Accomplishment: Quasi-Static Test Setup and Procedures

- **Pre-condition cells (SOC setup).**
- **Secure the hardware in x-axis orientation.**
- **Begin data recording and initiate crush platen motion at 1 mm/sec**
- **Continue crush at a constant rate until one of the following occurs;**
  - A 100 mV drop in voltage – temporary suspension.
  - EUCAR>3 event is reached – end of test.
  - The hardware has been crushed to 85% of displacement or the fixture load limit is reached – end of test.



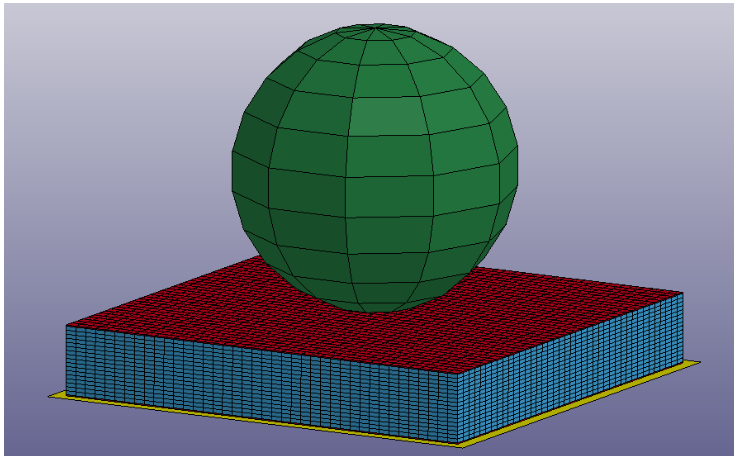
Initial trial: pouch material stick on the surface of indenter after a thermal event.

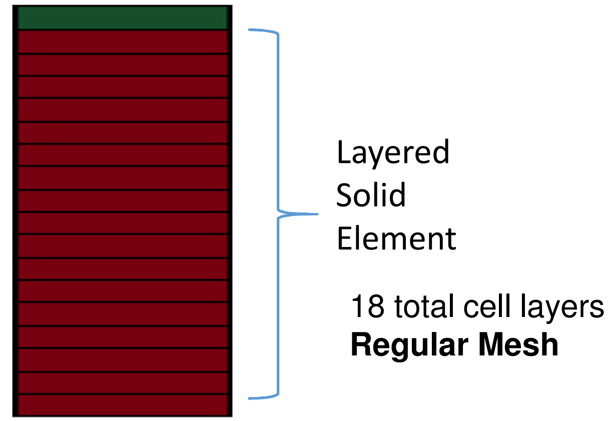


Boron nitride power coating (or cooking paper) applied to surface of indenter.

Go Further

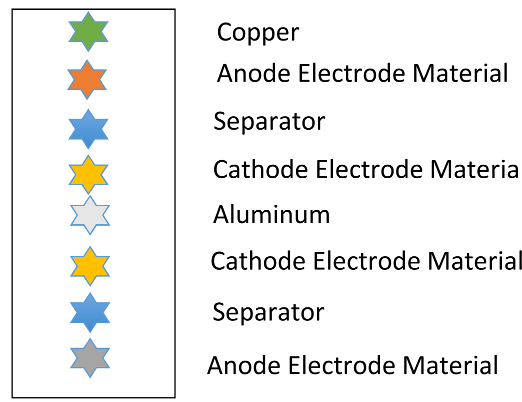
Technical Accomplishment: Quasi-Static Test with 75 mm Spherical Indenter and Flat Platen (Type D Cell)





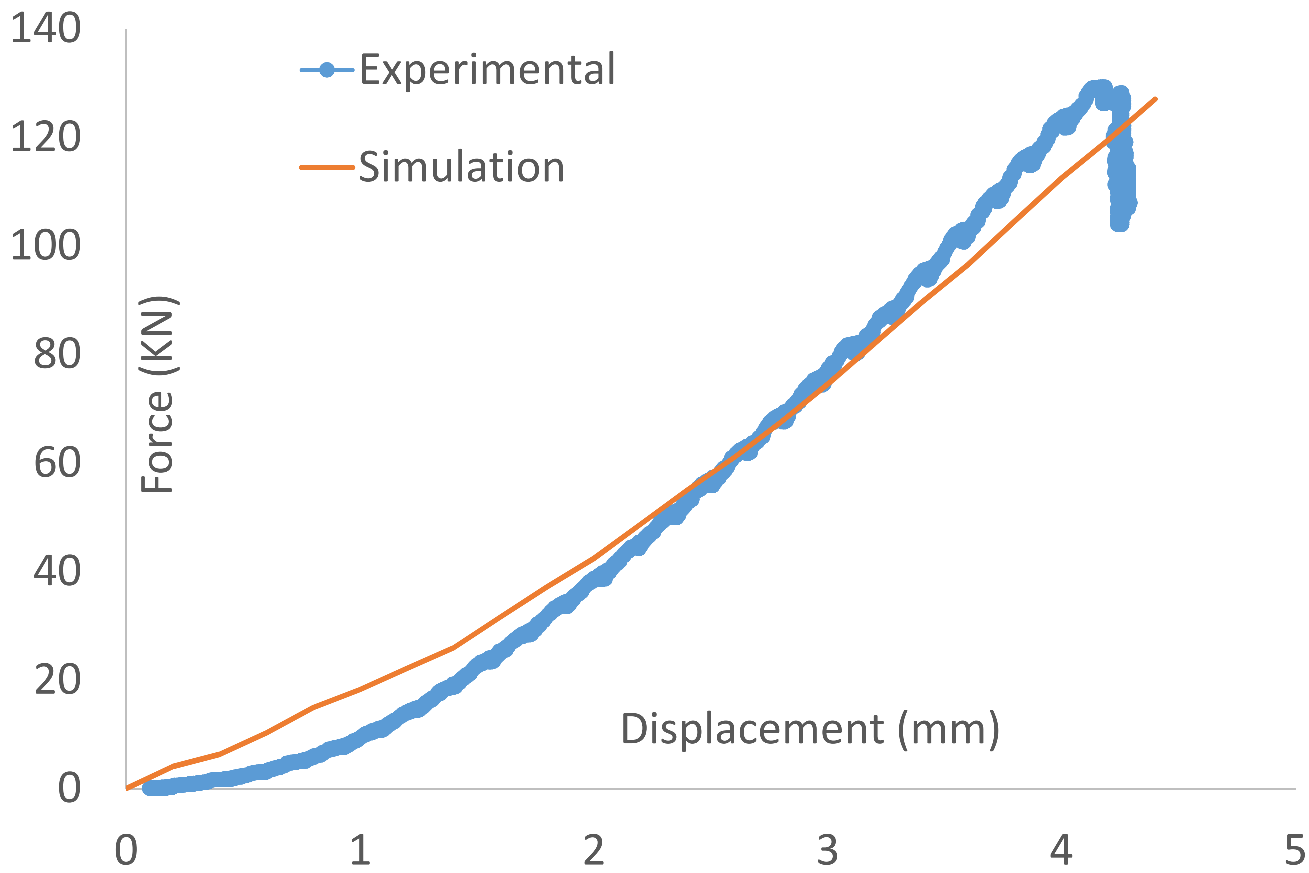
Component	Thickness (mm)	Material Model	Elastic Modulus (GPa)	Yield Strength (GPa)
Copper	0.011	MAT-24	110	0.24
Anode	0.064	MAT-63	0.45	0.04
Separator	0.024	MAT-24	0.5	0.06
Cathode	0.080	MAT-63	0.55	0.04
Aluminum	0.018	MAT-24	70	0.24

Layered Element Scheme



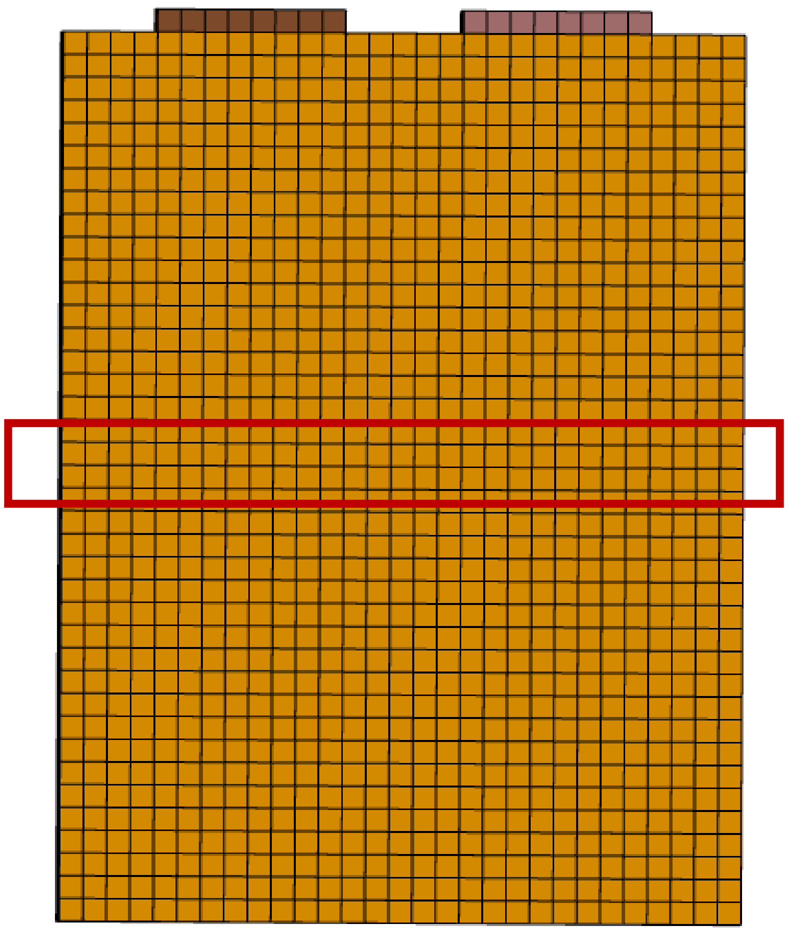
Go Further

Technical Accomplishment: Experimental vs. Simulation Quasi-Static Test with 75 mm Spherical Indenter and Flat Platen



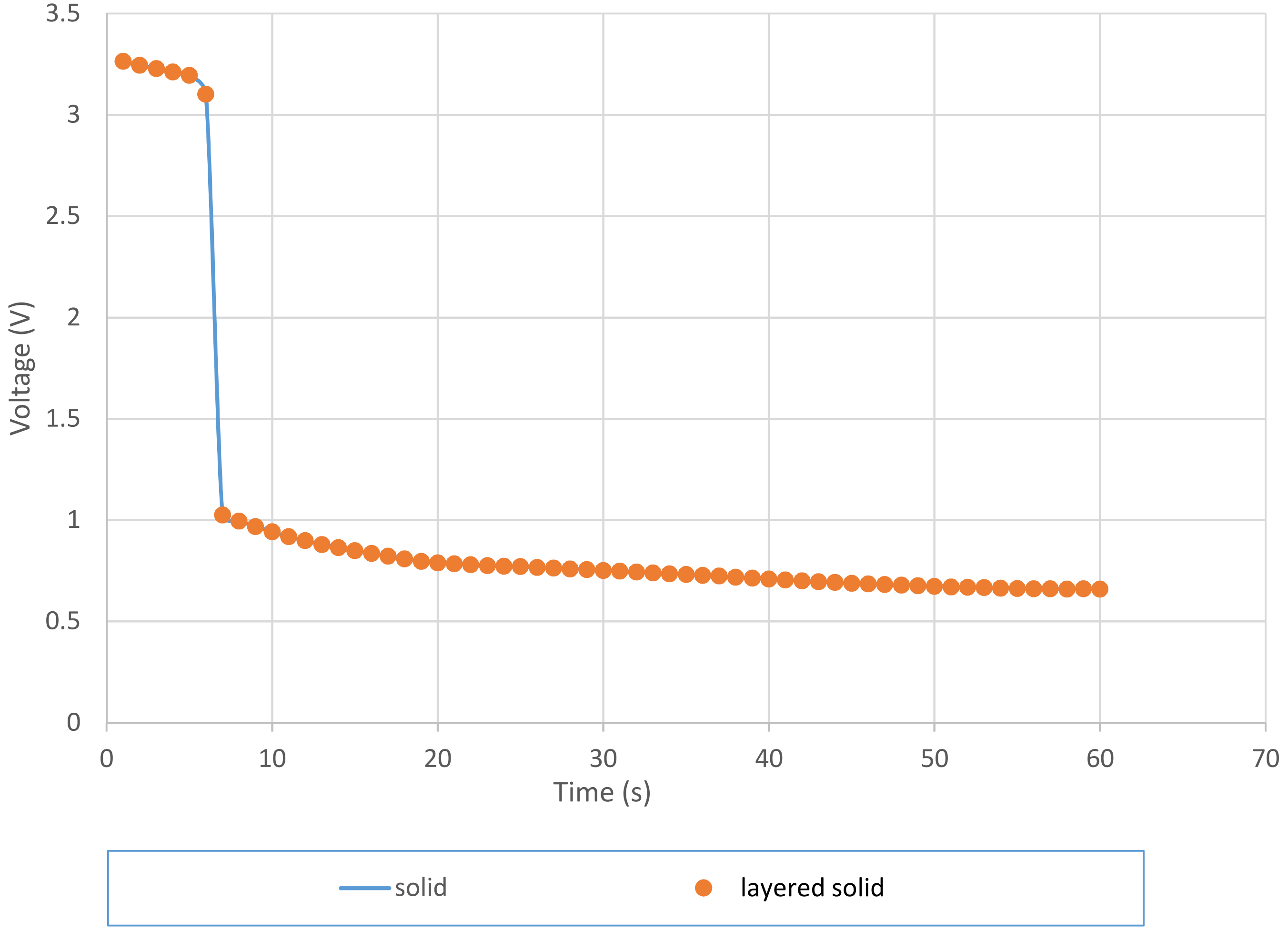
Go Further

Technical Accomplishment: Performance of Layered Solid Elements in EM and Thermal Solvers (Compression Mode)



- To mimic the scenario of internal short circuit, the resistance in the central part of the cell is large initially, and then drops rapidly after ~1s.
- The models involve EM and thermal solvers only. No mechanical deformation occurs in the simulation.

Technical Accomplishment: Comparison of cell voltage evolution



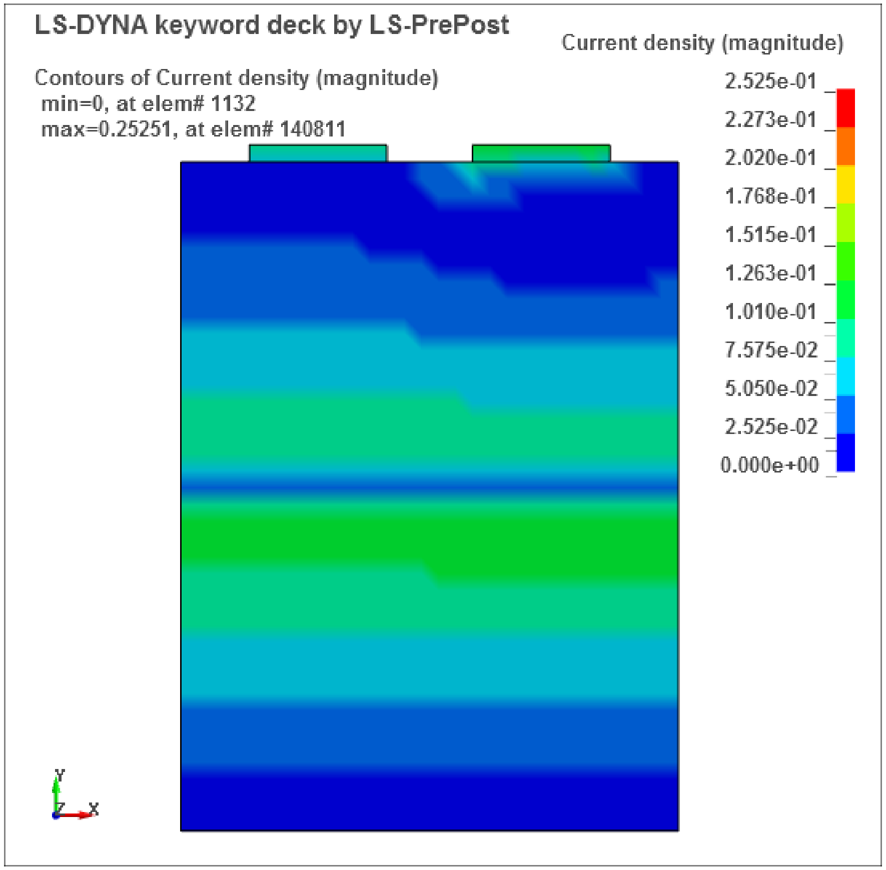
Go Further

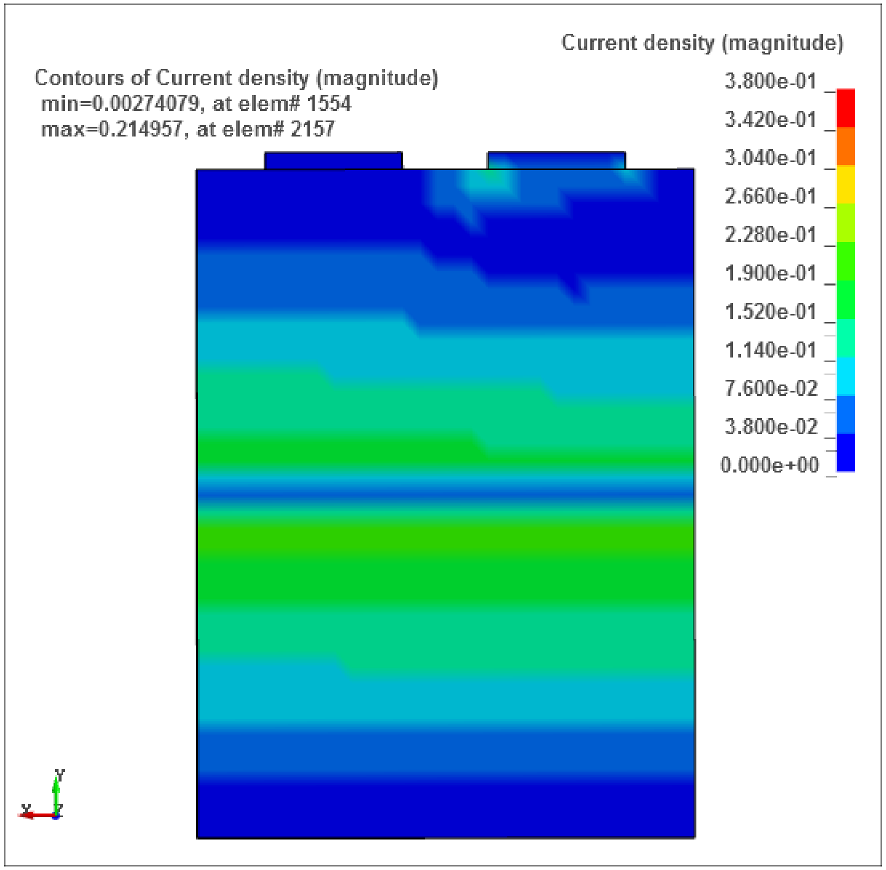
Technical Accomplishment: Comparison of current density distribution_Solid Element vs. Layered Solid Element

Standard solid elements

t = 10s

Layered solid elements





Go Further

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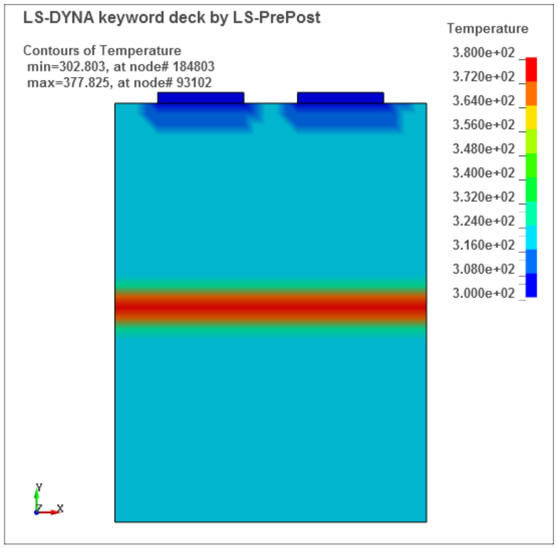
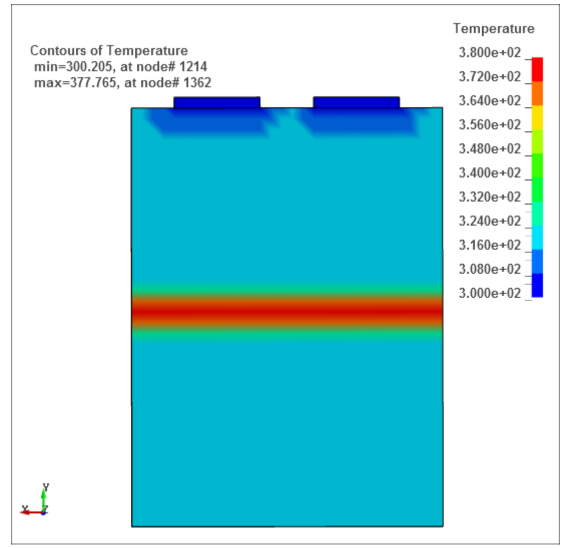
Technical Accomplishment: Comparison of Temperature Distribution_Solid Element vs. Layered Solid Element

Standard solid elements

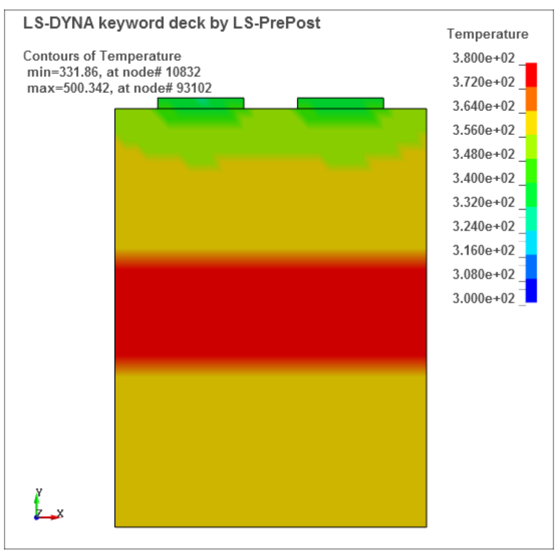
Layered solid elements

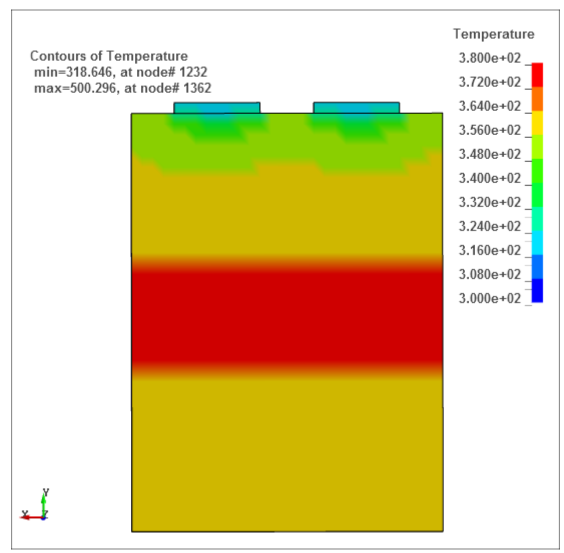
t = 10s





t = 20s





Go Further

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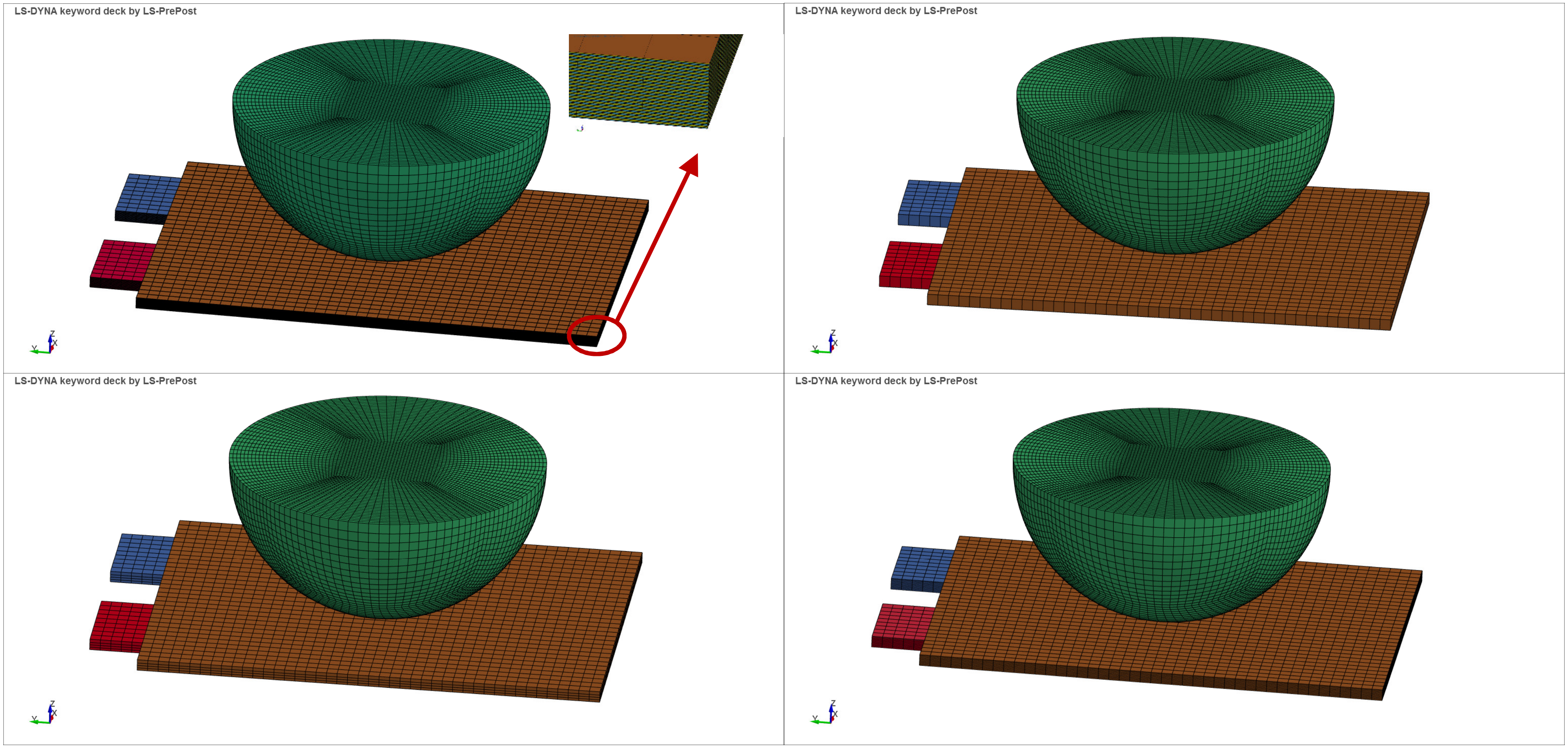
Technical Accomplishment: Performance of Layered Solid Elements (Indentation Mode)

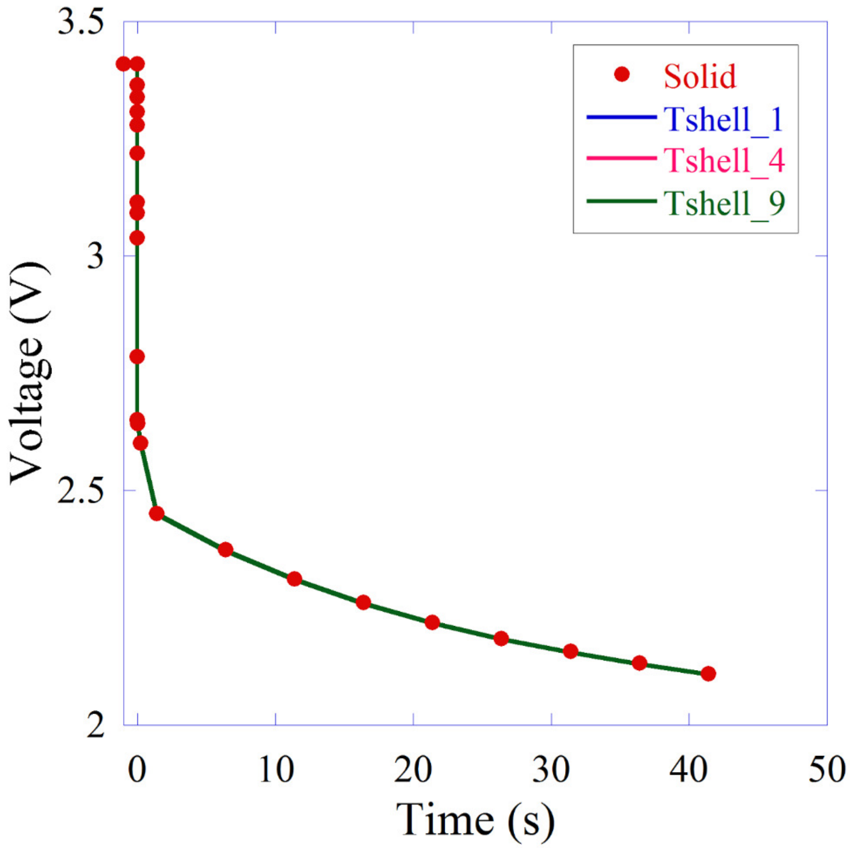


Models with standard solid elements and layered solid elements.
(= composite t-shell element: LS-Dyna definition of layered solid element), where the number of tshell elements in the thickness direction is 1, 4 and 9.

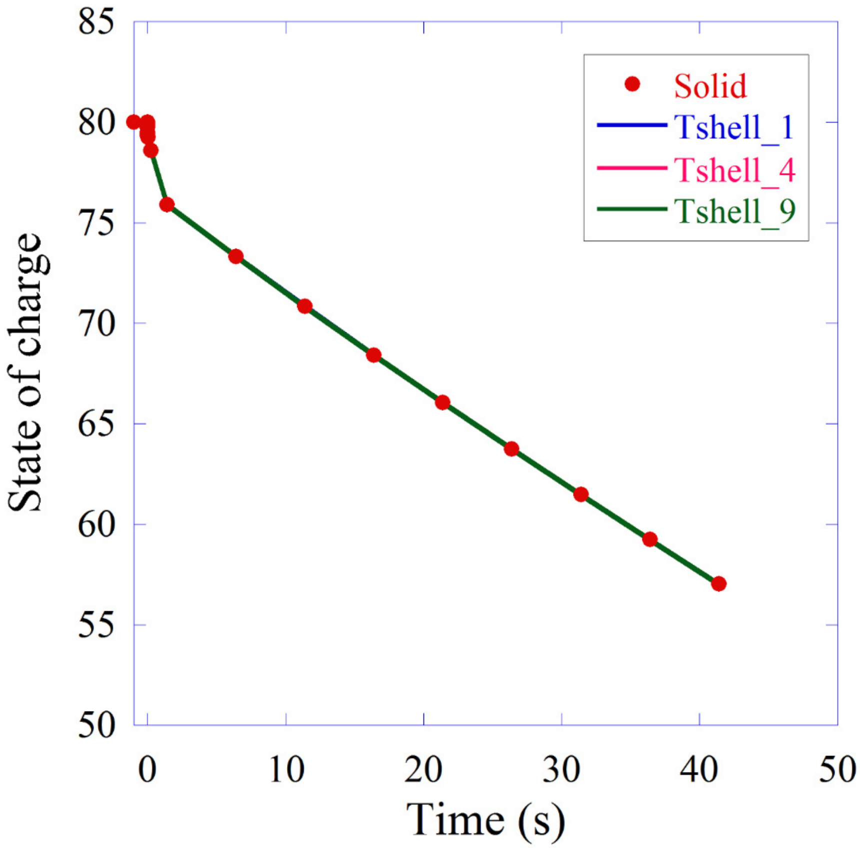
Go Further

Technical Accomplishment: Comparison of Cell Voltage and SOC Evolution (Solid Element vs. Layered Solid Element)

Cell voltage



State of charge



Go Further

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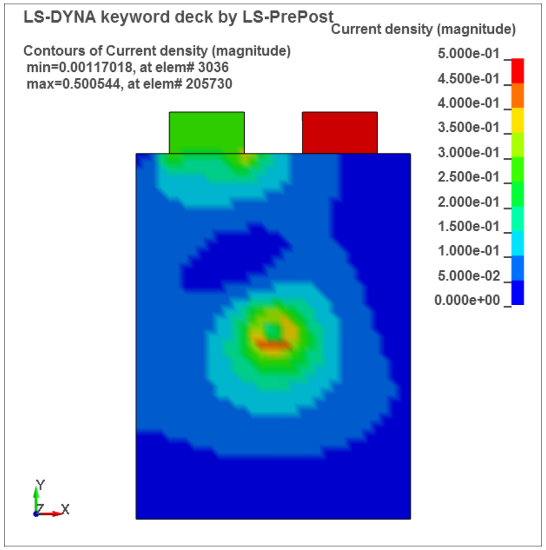
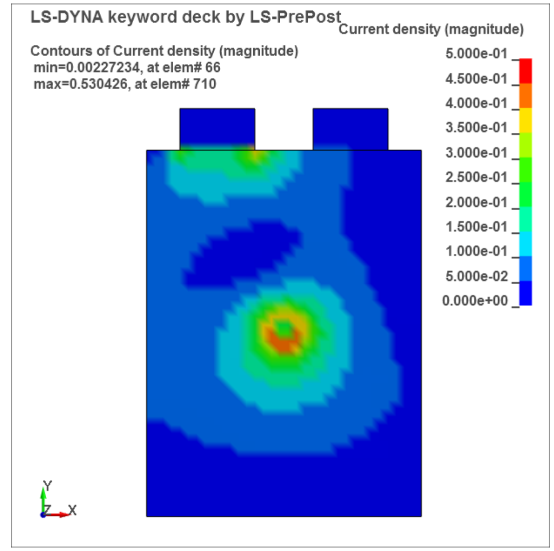
Technical Accomplishment: Comparison of Current Density Distribution at 41s

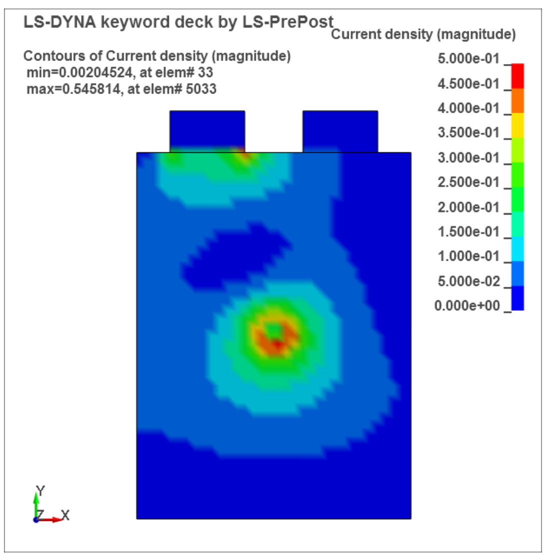
Solid



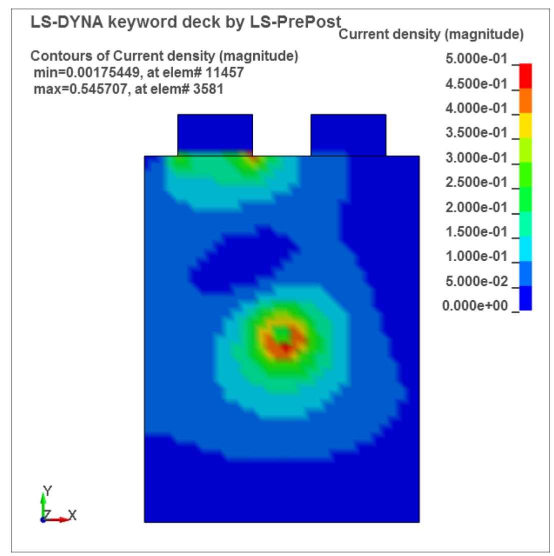
Tshell_1



Tshell_4

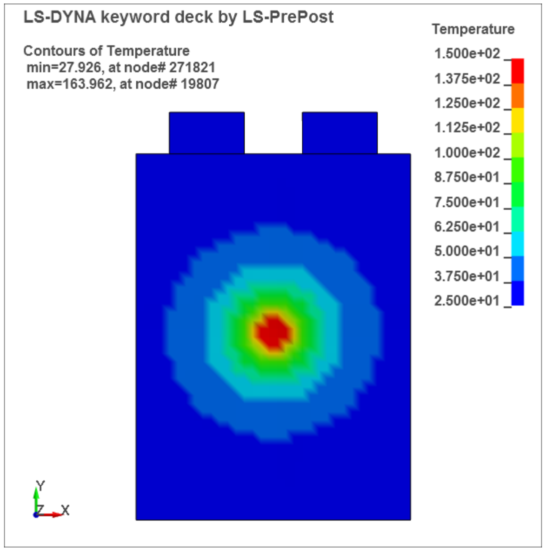


Tshell_9

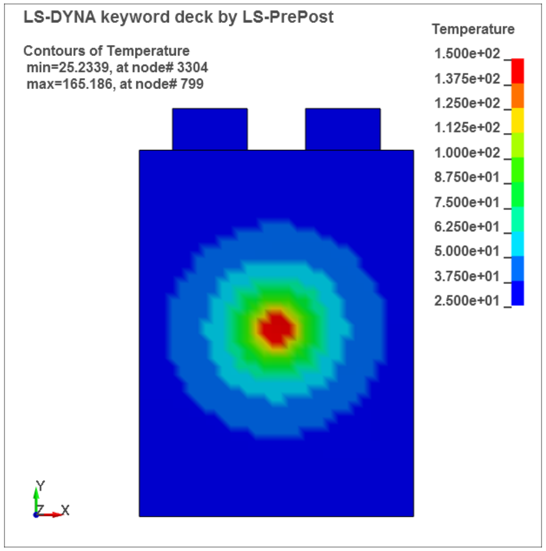


Technical Accomplishment: Comparison of Temperature Distribution at 41s

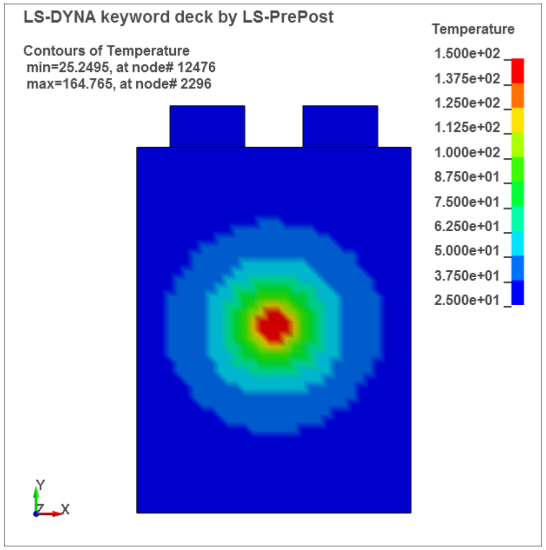
Solid



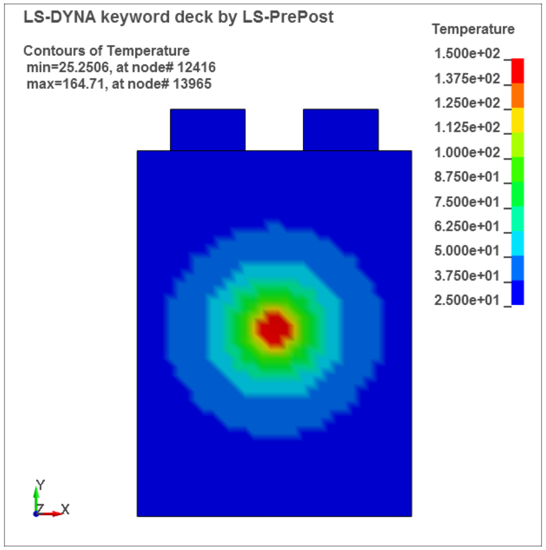
Tshell_1



Tshell_4



Tshell_9



Go Further

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Technical Accomplishment: Advantages of Using Layered Solid Element Solvers

- **Save time in the mechanical solver significantly.**
- **Achieve the same results in the mechanical, EM and thermal solvers so that the same mesh can be used by all solvers in a model.**
  - Save time in model development process (such as mesh, create Randles circuit models, …)
- **More numerically stable, in particular in the case of large deformation.**

Responses to Previous Reviewers' comments

- **Comment**
  - Which heat terms were included in the battery thermal model for this project?

- **Response**
  - Heat generation due to Joule heat, electrode reactions, and entropic heat generation are all considered in the thermal model of the α-version multi-physics model.

Collaborations and Coordination

- **ORNL is developing methods to scale-up detailed mechanical simulation to reduce computational complexity while retaining high fidelity.**
- **ORNL is also running X-Ray CT scan analyses to find the onset of crack formation and its growth on battery components during various mechanical deformations. This information will be used to establish the failure model of the battery.**

- **LS-DYNA® is the CAE software of choice for the project and contains key, battery-specific solver enhancements.**

Remaining Challenges and Barriers/ Future Research

- **Remaining Challenges and Barriers**
  - High speed impact testing is behind the original schedule due to lack of sophisticated equipment and resources at the supplier company.

- **Future Research**
  - The high speed impact tests will be run by an alternative supplier who has more experience and capability in terms of running crush tests.
  - Details on equipment and test schedule was finalized and the test rig was deigned and being built.
  - To catch the schedule, beta version validation test hardware (type D and type E battery modules) was secured ahead of the original schedule.
  - Another supplier was hired to run material analyses of the module components to run the beta version model validation tests.
  - Scale the simulation method to enable durability assessment of modules.
  - Development of a battery packaging module in LS-PREPOST to help users set up cases.

Summary

- **Delivery of α-version model**
  - Delivery of electrochemical and thermal models for Type D and Type E cells.
  - Created the multi-physics solvers (layered solid element formulation) with various material models.
  - Integrated the solvers into the α-version model.
  - Carried out shear stress and quasi-static tests to verify the multi-physics solvers under various cell-deformation modes.
    - Demonstrated that the layered solid element solver provided with the same results with much less computational time compared to the proven solid element solver.
  - Performed the X-ray CT scan analyses to define the failure condition that triggers internal short circuit and to develop the damage and failure models inside the layered solid element.

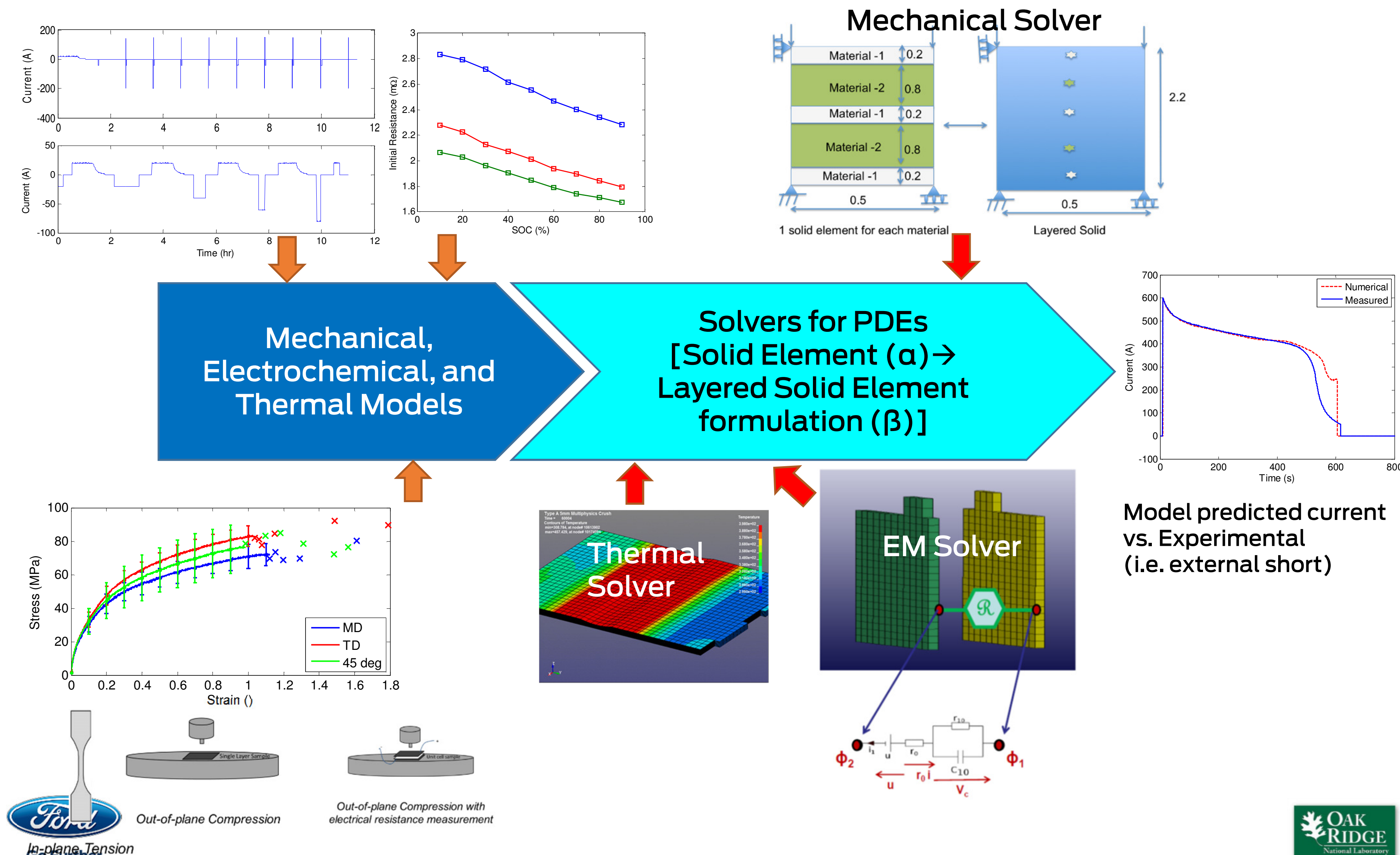
- **Development of β-version model**
  - Selected and secured the hardware for β-version model development.
  - Initiated development of the meshless Randles-circuit model for β-version model.

Go Further

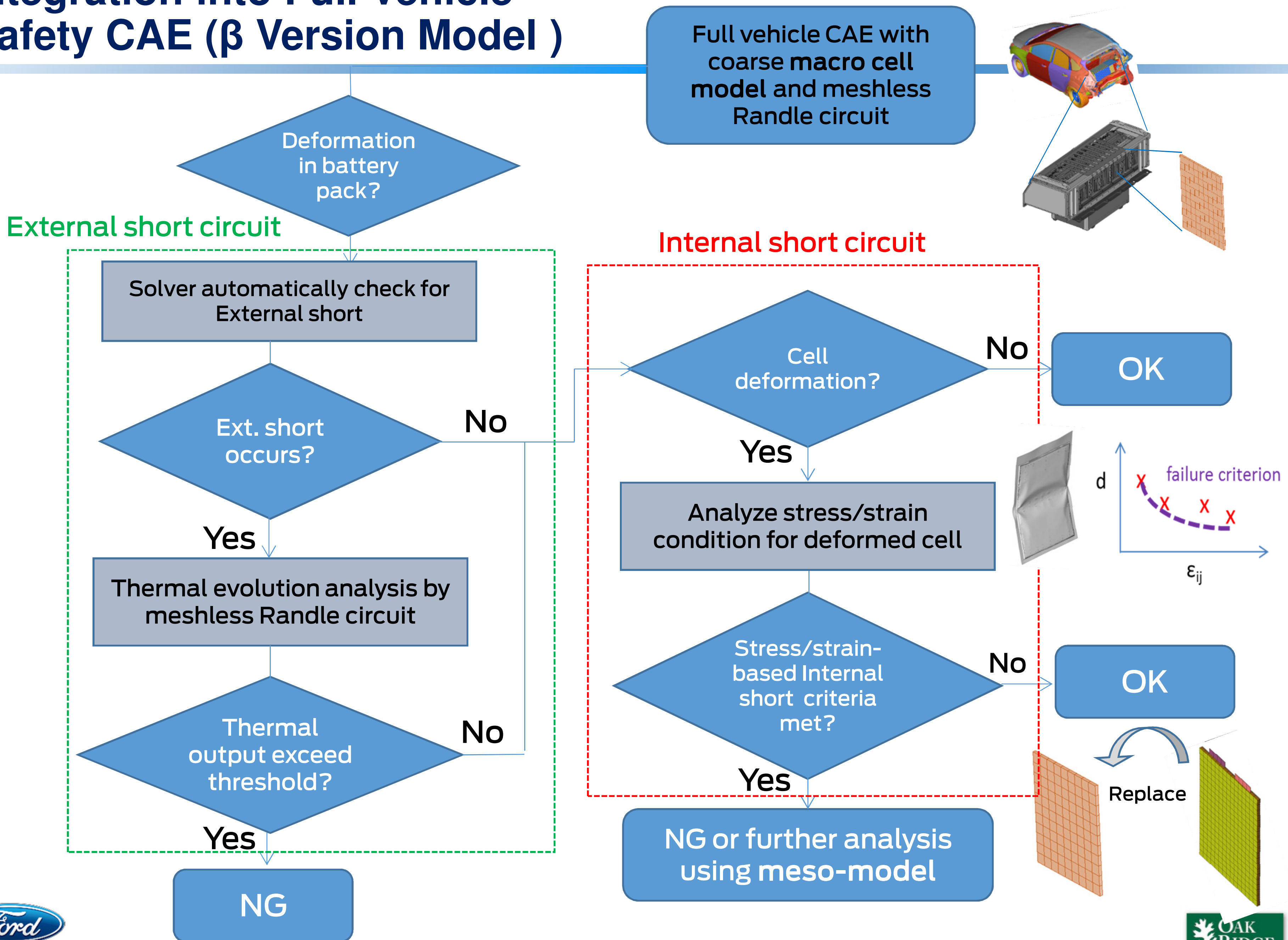
Technical Backup Slides

Go Further

Approach – α Version Model Development Overview



Integration into Full Vehicle Safety CAE (β Version Model)



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